Dedicated to Professor Bambi Hu in honor of his 60th birthday, with appreciation and love – Bei-Lok

Stochastic Gross-Pitaevsky Equation for BEC via Coarse-Grained Effective Action

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We sketch the major steps in a functional integral derivation of a new set of Stochastic Gross-Pitaevsky equations (GPE) for a Bose-Einstein condensate (BEC) confined to a trap at zero temperature with the averaged effects of non-condensate modes incorporated as stochastic sources. The closed-time-path (CTP) coarse-grained effective action (CGEA) or the equivalent influence functional method is particularly suitable because it can account for the full back-reaction of the noncondensate modes on the condensate dynamics self-consistently. The Langevin equations derived here containing nonlocal dissipation together with colored and multiplicative noises are useful for a stochastic (as distinguished from say, a kinetic) description of the nonequilibrium dynamics of a BEC. This short paper contains original research results not yet published anywhere.

I. INTRODUCTION

Two major paradigms are commonly adopted in describing the nonequilibrium dynamics of a many-body system. One is by way of kinetic theory [1, 2] based on the Boltzmann equation and its generalizations, which evolve the lowest order correlation functions (in the BBGKY hierarchy). The other captures the stochastic and dissipative dynamics of an open system, with the environment functioning as sources of noise with specific features determined from first principles, not put in by hand; and their overall effect engendering dissipation in the open system dynamics. Usually for a system well discernible from and whose effects dominate over its environment (the condensate is an open system with the noncondensate as its environment), the stochastic dynamics is often an easier and perhaps cleaner approach. Thus explains the great interest in deriving reliable stochastic equations for BEC dynamics.

For BEC stochastic dynamics, historically Gardiner and his co-workers [3] were the first to derive a set of stochastic Gross-Pitaevsky equations. Their method combines the kinetic theory and the open systems approaches. We present here an alternative derivation via the closed-time-path (CTP) [4] coarse-grained effective action (CGEA) [5] or the closely related influence functional [6] method. This method has the merit that it can account for the full back-reaction of the noncondensate modes on the condensate dynamics self-consistently. Our results are structurally similar to theirs but the content is more complex: Our Langevin equations contains nonlocal dissipation and colored and multiplicative noises. These two kernels provide all the necessary information for a stochastic description of the nonequilibrium dynamics of a BEC. [8]

II. QUANTUM FIELD THEORY OF BEC DYNAMICS

For a field-theoretic description of BEC we begin with a second - quantized field operator $\Psi(\vec{x},t)$ which removes an atom at the location $\vec{x}$ at times t. It obeys canonical commutation relations

$$[\Psi(\vec{x},t), \Psi(\vec{y},t)] = 0, \tag{1}$$

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$$\left[\Psi\left(\vec{x},t\right),\Psi^{\dagger}\left(\vec{y},t\right)\right]=\delta\left(\vec{x}-\vec{y}\right). \tag{2}$$

The dynamics of this field is given by the Heisenberg equations of motion (we choose units such that $\hbar=1$)

$$-i\frac{\partial}{\partial t}\Psi=\left[\mathbf{H},\Psi\right], \tag{3}$$

where $\mathbf{H}$ is the Hamiltonian. The theory is invariant under a global phase change of the field operator

$$\Psi\rightarrow e^{i\theta}\Psi,\qquad \Psi^{\dagger}\rightarrow e^{-i\theta}\Psi^{\dagger}. \tag{4}$$

The constant of motion associated with this invariance through Noether's theorem is the total particle number.

We shall consider only the simplest Hamiltonian

$$\mathbf{H}=\int d^{d}\vec{x}\,\left\{\Psi^{\dagger}H\Psi+\frac{U}{2}\Psi^{\dagger 2}\Psi^{2}\right\}, \tag{5}$$

where we have reduced the atom - atom interactions to a single contact potential with a delta-like repulsion term. The coupling constant U is often parameterized in terms of the scattering length a and the mass M of the atom as $U=4\pi a/M$. The single - particle Hamiltonian H is given by

$$H\Psi=-\frac{1}{2M}\nabla^{2}\Psi+V_{trap}\left(\vec{x}\right)\Psi, \tag{6}$$

$V_{trap}\left(\vec{x}\right)$ denotes a confining trap potential. Then the Heisenberg equation of motion

$$i\frac{\partial}{\partial t}\Psi=H\Psi+U\Psi^{\dagger}\Psi^{2}, \tag{7}$$

is also the classical equation of motion derived from the action

$$S=\int dt\;d^{d}x\;i\Psi^{*}\frac{\partial}{\partial t}\Psi-\int dt\;\mathbf{H}. \tag{8}$$

III. CONDENSATE AS OPEN SYSTEM

We adopt the quantum open system framework and define our system of condensate as comprising a superposition of only a few low lying modes of the one-particle Hamiltonian. The condensate while evolving can excite the quantum fluctuations in the higher modes, which in turn back-react on the condensate, thus modifying its test-field dynamics (i.e, that which is obtained without backreaction). We regard the condensate as an open system living in the environment provided by the higher modes and try to incorporate the effects of the coarse-grained environment in some way. The inclusion of backreaction effects in our experience is best performed via the coarse grained effective action or the influence functional as they ensure full self-consistency.

We first partition the total wave function into the system sector and an environment sector. We do this by way of projection operators. Assume a complete set of one-particle states

$$H\psi_{\alpha}\left(\vec{x}\right)=\omega_{\alpha}\psi_{\alpha}\left(\vec{x}\right). \tag{9}$$

Choose an appropriate partition frequency ω_{C} and define two projectors

$$\mathcal{P}=\sum_{\omega_{\alpha}\leq\omega_{C}}\psi_{\alpha}\left(\vec{x}\right)\psi_{\alpha}\left(\vec{x}'\right), \tag{10}$$

which projects onto the low lying modes (band) comprising the condensate, our system, and

$$\mathcal{Q}=\delta\left(\vec{x}-\vec{x}'\right)-\mathcal{P}. \tag{11}$$

which projects onto the sector of higher modes, the noncondensate, constituting an environment for the system. Define the condensate band field operator

$$\phi\left(t,\vec{x}\right)=\mathcal{P}\Psi\left(t,\vec{x}\right), \tag{12}$$

and split

$$\Psi\left(t,\vec{x}\right)=\phi\left(t,\vec{x}\right)+\chi\left(t,\vec{x}\right). \tag{13}$$

Here, ϕ denotes the *quantum* wave function of the condensate, not a c-number wave function usually assumed.

We now split the action into condensate (C), non-condensate (NC) and interaction (int) parts

$$S\left[\phi+\chi\right]=S_C\left[\phi\right]+S_{NC}\left[\chi\right]+S_{int}\left[\phi,\chi\right]. \tag{14}$$

The first two are just the full action evaluated at the corresponding field. S_{int} may be written as the sum of three terms in successive higher powers of the noncondensate operator:

$$S_{int}=S_1+S_2+S_3, \tag{15}$$

with

$$S_1=-U\int dt\, d^d\vec{x}\ \left\{\phi^{\dagger 2}\phi\chi+\chi^{\dagger}\phi^{\dagger}\phi^2\right\}, \tag{16}$$

$$S_2=-\frac{U}{2}\int dt\, d^d\vec{x}\ \left\{\phi^{\dagger 2}\chi^2+\chi^{\dagger 2}\phi^2+4\phi\phi\chi^{\dagger}\chi\right\}, \tag{17}$$

$$S_3=-U\int dt\, d^d\vec{x}\ \left\{\phi^{\dagger}\chi^{\dagger}\chi^2+\chi^{\dagger 2}\chi\phi\right\}, \tag{18}$$

where $\phi^{\dagger}$ is the hermitian conjugated field of ϕ. To simplify the appearances we represent the pair $\left(\phi,\phi^{\dagger}\right)$ as the up and down components (respectively) of a spinor ϕ^a, $a=1,2$, and adopt the DeWitt convention where the space-time arguments are assumed to be included in the spinor indices.

IV. CGEA AND STOCHASTIC GROSS-PITAEVSKY (LANGEVIN) EQUATION

We now introduce the coarse-grained effective action. Assume for simplicity that at $t=0$ the quantum state of the gas is described by a factorizable density matrix

$$\rho\left[\phi^1+\chi^1,\phi^2+\chi^2,0\right]=\rho_C\left[\phi^1,\phi^2,0\right]\rho_{NC}\left[\chi^1,\chi^2,0\right]. \tag{19}$$

The expectation values of field operators may be derived from the usual closed time-path (CTP) generating functional

$$exp\left\{iW\left[J^1,J^2\right]\right\}=\int D\Psi^1\, D\Psi^2\ e^{i\left(S\left[\Psi^1\right]-S\left[\Psi^2\right]+\int dt\, d^dx\ \left[J^1\Psi^1-J^2\Psi^2\right]\right)}\rho\left(0\right). \tag{20}$$

However, if we are interested in the expectation values of the condensate band operators, then we only need to couple sources to these fields, namely

$$\mathcal{Q}J^{1,2}=0. \tag{21}$$

The integral over non-condensate fields may be performed, and we obtain the condensate generating functional

$$exp\left\{iW_C\left[J^1,J^2\right]\right\}=\int D\phi^1\, D\phi^2\ e^{i\left(S_{CGEA}\left[\phi^1,\phi^2\right]+\int dt\, d^dx\ \left[J^1\phi^1-J^2\phi^2\right]\right)}\rho_C\left(0\right), \tag{22}$$

where the coarse-grained effective action is

$$S_{CGEA}\left[\phi^1,\phi^2\right]=S_C\left[\phi^1\right]-S_C\left[\phi^2\right]+S_{IF}\left[\phi^1,\phi^2\right], \tag{23}$$

where S_{IF} is the influence action and

$$exp\left\{iS_{IF}\left[\phi^1,\phi^2\right]\right\}=\int D\chi^1\, D\chi^2\ e^{i\left(S_{NC}\left[\chi^1\right]+S_{int}\left[\phi^1,\chi^1\right]-S_{NC}\left[\chi^2\right]-S_{int}\left[\phi^2,\chi^2\right]\right)}\rho_{NC}\left(0\right). \tag{24}$$

is the influence functional (IF).

To make the physical content of the CGEA more explicit, it is convenient to introduce new field variables

$$\phi_+ = \frac{1}{2}\left(\phi^1 + \phi^2\right), \quad \phi_- = \phi^1 - \phi^2. \tag{25}$$

If we Taylor expand S_{CGEA} in powers of ϕ_- we find that there is no independent term, and that even terms are imaginary and odd terms are real. The path integral (22) admits a saddle point with respect to ϕ_- at $\phi_- = 0$. We concentrate on the contribution of field configurations near this saddle point by keeping only quadratic terms in ϕ_- in the CGEA

$$\begin{aligned} S_{IF}\left[\phi_+,\phi_-\right] &= \int dt\, d^d\vec{x}\, \mathcal{D}_a\left[\phi_+\right]\phi_-^a \\ &+ \frac{i}{2}\int dt\, d^d\vec{x}\int dt'\, d^d\vec{x}'\, \mathcal{N}_{ab}\left[\phi_+\right]\phi_-^a\phi_-^b + \dots \end{aligned} \tag{26}$$

To get an explicit representation, we introduce the functional expectation value

$$\langle A\rangle\left[\phi_+\right] = \int D\chi^1\, D\chi^2\, e^{i\left(S_{NC}\left[\chi^1\right]+S_{int}\left[\phi_+,\chi^1\right]-S_{NC}\left[\chi^2\right]-S_{int}\left[\phi_+,\chi^2\right]\right)}A\rho_{NC}\left(0\right). \tag{27}$$

Then

$$\mathcal{D}_a\left[\phi_+\right] = \frac{\delta S_C}{\delta\phi_+^a} + \frac{1}{2}\left\langle\frac{\delta S_{int}}{\delta\phi_+^a}\left[\phi_+,\chi^1\right] + \frac{\delta S_{int}}{\delta\phi_+^a}\left[\phi_+,\chi^2\right]\right\rangle\left[\phi_+\right], \tag{28}$$

and

$$\begin{aligned} \mathcal{N}_{ab}\left[\phi_+\right] &= \frac{-i}{4}\left\langle\frac{\delta^2 S_{int}}{\delta\phi_+^a\delta\phi_+^b}\left[\phi_+,\chi^1\right] - \frac{\delta^2 S_{int}}{\delta\phi_+^a\delta\phi_+^b}\left[\phi_+,\chi^2\right]\right\rangle\left[\phi_+\right] \\ &+ \frac{1}{4}\left\langle\left\{\frac{\delta S_{int}}{\delta\phi_+^a}\left[\phi_+,\chi^1\right] + \frac{\delta S_{int}}{\delta\phi_+^a}\left[\phi_+,\chi^2\right]\right\}\left\{\frac{\delta S_{int}}{\delta\phi_+^b}\left[\phi_+,\chi^1\right] + \frac{\delta S_{int}}{\delta\phi_+^b}\left[\phi_+,\chi^2\right]\right\}\right\rangle\left[\phi_+\right] \\ &- \frac{1}{4}\left\langle\frac{\delta S_{int}}{\delta\phi_+^a}\left[\phi_+,\chi^1\right] + \frac{\delta S_{int}}{\delta\phi_+^a}\left[\phi_+,\chi^2\right]\right\rangle\left[\phi_+\right]\left\langle\frac{\delta S_{int}}{\delta\phi_+^b}\left[\phi_+,\chi^1\right] + \frac{\delta S_{int}}{\delta\phi_+^b}\left[\phi_+,\chi^2\right]\right\rangle\left[\phi_+\right]. \end{aligned} \tag{29}$$

From here one can deduce that generally a representation

$$\mathcal{N}_{ab}\left[\phi_+\right] = \sum_{ij}\nu_{ac,bd}^{ij}f_i^c\left[\phi_+\right]f_j^d\left[\phi_+\right], \tag{30}$$

can be obtained in terms of a set of local functionals f_i^a. This allows us to rewrite the condensate generating functional as

$$\begin{aligned} exp\left\{iW_C\left[J_+,J_-\right]\right\} &= \int D\xi_{ac}^i\,\Upsilon\left[\xi_{ac}^i\right]\, D\phi_+\, D\phi_-\, e^{i\int dt\, d^dx\, J_-\phi_+} \\ &\qquad e^{i\int dt\, d^dx\,\left\{\mathcal{D}_a\left[\phi_+\right]+\sum_i\xi_{ac}^i f_i^c\left[\phi_+\right]+J_+\right\}\phi_-^a}\rho_C\left(0\right), \end{aligned} \tag{31}$$

where the Feynman-Vernon trick of using a Gaussian functional identity [6] involving the stochastic distribution Υ is invoked. Here

$$J_+ = \frac{1}{2}\left(J^1 + J^2\right), \quad J_- = J^1 - J^2, \tag{32}$$

and the ξ_{ac}^i are the Gaussian stochastic sources with zero mean and cross correlation

$$\left\langle\xi_{ac}^i\xi_{bd}^j\right\rangle = \nu_{ac,bd}^{ij}. \tag{33}$$

It should be noted that the stochastic terms do not appear explicitly, but only implicitly in the form of random contribution to the action, which then is averaged over. However, performing the final integration over ϕ_-^a we see that the only contributions to the path integral come from condensate field configurations which obey the equation

$$\mathcal{P}\left\{\mathcal{D}_a\left[\phi_+\right] + \sum_i\xi_{ac}^i f_i^c\left[\phi_+\right] + J_+\right\} = 0, \tag{34}$$

with random initial conditions weighted by the Wigner function constructed from the initial density matrix $\rho_C(0)$. The free evolution of the condensate is obtained by setting $J_+ = 0$. In this sense, the condensate field evolves as an ensemble of trajectories, each obeying the stochastic Langevin-type equation (34). This is a consequence of the truncation of S_{CGEA} to just quadratic terms in ϕ_-^a. Further terms in S_{CGEA} would introduce effects associated to the quantum nature of the condensate field. The presence of the projection operator $\mathcal{P}$ in (34) enforces the consistency of the system - environment split under time evolution.

We observe that because of the nonlocal terms in $\mathcal{D}_a$ this equation is generally dissipative and contain noises which are generally colored because of the nonlocality of the cross correlations $\nu_{ac,bd}^{ij}$, and multiplicative because of nonlinearity in the f_i^c. There ought to be a fluctuation-dissipation relation for each types of the noise. A similar description for a theory with polynomial type of system-environment coupling can be found in Hu, Paz and Zhang (1993) of [6]; see also [7].

V. DISSIPATION AND NOISE KERNELS

We can glean more physical meanings about dissipation and fluctuations by trying to obtain more explicit expressions for these kernels. We go back to our model of a gas confined in a time-independent trap, and compute the CGEA to order U^2 at zero temperature ($T = 0$) for the vacuum. We obtain (from here on, to simplify appearances, we drop the + subindex on ϕ_+)

$$\begin{aligned}
\mathcal{D}_a[\phi] &= \frac{\delta S_C}{\delta\phi^a} + \frac{iU^2}{2}\int^t dt' d\vec{x}' \\
&\quad \left\{ \frac{\partial\phi^{\dagger 2}\phi}{\partial\phi^a}(t,\vec{x})\; F^+(t-t',\vec{x},\vec{x}')\,\phi^\dagger\phi^2(t',\vec{x}') \right. \\
&- \frac{\partial\phi^\dagger\phi^2}{\partial\phi^a}(t,\vec{x})\,F^-(t-t',\vec{x},\vec{x}')\,\phi^{\dagger 2}\phi(t',\vec{x}') \\
&+ \frac{1}{2}\frac{\partial\phi^{\dagger 2}}{\partial\phi^a}(t,\vec{x})\,F^{+2}(t-t',\vec{x},\vec{x}')\,\phi^2(t',\vec{x}') \\
&- \left. \frac{1}{2}\frac{\partial\phi^2}{\partial\phi^a}(t,\vec{x})\,F^{-2}(t-t',\vec{x},\vec{x}')\,\phi^{\dagger 2}(t',\vec{x}') \right\},
\end{aligned} \tag{35}$$

where

$$\begin{aligned}
F^+(t-t',\vec{x},\vec{x}') &= \left\langle \chi(t,\vec{x})\,\chi^\dagger(t',\vec{x}') \right\rangle \\
&= \sum_{\omega_\alpha > \omega_C} e^{-i\omega_\alpha(t-t')}\psi_\alpha(\vec{x})\,\psi_\alpha(\vec{x}'),
\end{aligned} \tag{36}$$

$$\begin{aligned}
F^-(t-t',\vec{x},\vec{x}') &= \left\langle \chi(t',\vec{x}')\,\chi^\dagger(t,\vec{x}) \right\rangle \\
&= \sum_{\omega_\alpha > \omega_C} e^{i\omega_\alpha(t-t')}\psi_\alpha(\vec{x})\,\psi_\alpha(\vec{x}').
\end{aligned} \tag{37}$$

With respect to the noise terms, we find that they may be represented in terms of four stochastic terms ζ^1 to ζ^4

$$\xi_{ac}^i = \delta_{ac}\zeta^i,\ \ i = 1,\ldots,4, \tag{38}$$

coupled to four functions f_1 to f_4

$$f_{1a} = \frac{1}{2}\frac{\partial}{\partial\phi^a}\left[\phi^{\dagger 2}\phi + \phi^\dagger\phi^2\right], \tag{39}$$

$$f_{2a} = \frac{-i}{2}\frac{\partial}{\partial\phi^a}\left[\phi^{\dagger 2}\phi - \phi^\dagger\phi^2\right], \tag{40}$$

$$f_{3a} = \frac{1}{2}\frac{\partial}{\partial\phi^a}\left[\phi^{\dagger 2} + \phi^2\right], \tag{41}$$

$$f_{4a} = \frac{-i}{2} \frac{\partial}{\partial \phi^a} \left[\phi^{\dagger 2} - \phi^2 \right]. \tag{42}$$

The nontrivial cross correlations are

$$\left\langle \zeta^1 (t, \vec{x}) \, \zeta^1 (t', \vec{x}') \right\rangle = \left\langle \zeta^2 (t, \vec{x}) \, \zeta^2 (t', \vec{x}') \right\rangle = \frac{1}{2} F_p (t - t', \vec{x}, \vec{x}'), \tag{43}$$

$$\left\langle \zeta^1 (t, \vec{x}) \, \zeta^2 (t', \vec{x}') \right\rangle = \frac{i}{2} F_m (t - t', \vec{x}, \vec{x}'), \tag{44}$$

$$\left\langle \zeta^3 (t, \vec{x}) \, \zeta^3 (t', \vec{x}') \right\rangle = \left\langle \zeta^4 (t, \vec{x}) \, \zeta^4 (t', \vec{x}') \right\rangle = \mathbf{F}_p (t - t', \vec{x}, \vec{x}'), \tag{45}$$

$$\left\langle \zeta^3 (t, \vec{x}) \, \zeta^4 (t', \vec{x}') \right\rangle = i \mathbf{F}_m (t - t', \vec{x}, \vec{x}'), \tag{46}$$

where

$$F_p = F^+ + F^-, \quad F_m = F^+ - F^-, \quad \mathbf{F}_p = F^{+2} + F^{-2}, \quad \mathbf{F}_m = F^{+2} - F^{-2}. \tag{47}$$

The detailed forms of the noise and dissipation kernels in the stochastic Gross-Pitaevsky (Langevin) equation are useful for a comprehensive and in-depth study of the stochastic dynamics of the condensate incorporating its interaction with the noncondensates. Various aspects of this problem are understudy and results will be reported elsewhere.

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